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REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	12-14-00	Final Report (7/1/96-6/30/00)

4. TITLE AND SUBTITLE
Research in Nonlinear Material Behavior

5. FUNDING NUMBERS
DAAH04-96-1-0060

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8. PERFORMING ORGANIZATION REPORT NUMBER
DAAH04/CNA/00

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U. S. Army Research Office
P. O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
ARO 35219.3-CI

11. SUPPLEMENTARY NOTES
The view, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy, or decision, unless so designated by other documentation.

12a. DISTRIBUTION/AVAILABILITY STATEMENT
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12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

The focus of Greenberg's and Kinderlehrer's activities are the behavior of nonlinear material systems at widely varying length and time scales and in many different environments. The specific areas ccvered in this research were shallow water waves, metastable systems, in particular, melt-solidification problems using phase-field models, traffic modelling, simulation of hysteresis and its analysis in magnetic and manetoelastic systems, mesoscale properties of polycrystalline materials with focus on the development of new techniques to resolve the grain boundary energy from experimental information, and the mesoscale simulation of grain growth.

14. SUBJECT TERMS
metastable systems, mesoscale, multiscale phenomena, magnetic systems, shallow water waves, melt-solidicication, traffic modelling, hysteresis, magnetic systems polycrystalline materials

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. 239-18
298-102

DAAH04-96-10060 Final Report

(1) Foreward

The focus of Greenberg's and Kinderlehrer's activities are the behavior of nonlinear material systems at widely varying length and time scales and in many different environments.

(4) Main problems studied

Shallow water waves (Greenberg and Yershov)

Metastable systems, in particular, melt-solidification problems using phase-field models (Greenberg)

Traffic modelling (Greenberg)

Simulation of hysteresis and its analysis in magnetic and magnetoelastic systems (Kinderlehrer)

Mesoscale properties of polycrystalline materials with focus on the development of new techniques to resolve the grain boundary energy from experimental information (Kinderlehrer and Mason)

Mesoscale simulation of grain growth (Kinderlehrer and Livshits)

(5) Summary of the most important results

Shallow water waves

Shallow water equations with variable bottom topography and related work on conservation laws with source terms [1-3]. These studies have involved developing numerical algorithms which account for the source terms and have the same equilibrium structure as the underlying partial differential equations. Andrew Yershov, Greenberg's PhD student, and Greenberg have developed shock capturing Godunov codes for the shallow water equations (in two dimensions). This work was presented in a seminar at the Waterways Experimental Station in Vicksburg.
Metastable systems, in particular, melt-solidification problems using phase-field models

Greenberg has continued his work on meta-stable systems. A manuscript dealing with the behavior of melt-solidification problems using phase-field models has been completed and submitted to Mathematical Modelling and Numerical Analysis. A new set of *a priori* estimates have been obtained which allow one to make definitive predictions about the long-time asymptotics. He has also developed some robust algorithms to computationally handle these problems.

Metastable systems, in particular, melt-solidification problems using phase-field models

In a previous paper the author and Demay advanced a model to explain the melt fracture instability observed when molten linear polymer melts are extruded in a capillary rheometer operating under the controlled condition that the inlet flow rate was held constant. The model postulated that the melts were a slightly compressible viscous fluid and allowed for slipping of the melt at the wall. The novel feature of that model was the use of an empirical switch law which governed the amount of wall slip. The model successfully accounted for the oscillatory behavior of the exit flow rate, typically referred to as the melt fracture instability, but did not simultaneously yield the fine scale spatial oscillations in the melt typically referred to as shark skin.

In this note a new model is advanced which simultaneously explains the melt fracture instability and shark skin phenomena. The modelpostulates that the polymer is a slightly compressible linearly viscous fluid but assumes no slip boundary conditions at the capillary wall. In simple shear the shear stress τ and strain rate d are assumed to be related by $d = F\tau$ where F ranges between F_2 and $F_1 > F_2$. A strain rate dependent yield function is introduced and this function governs whether F evolves towards F_2 or F_1. This model accounts for the empirical observation that at high shears polymers align and slide more easily than at low shears and explains both the melt fracture and shark skin phenomena.

The results of this investigation appear in [8].

Traffic Modelling

In a recent paper Aw and Rascle introduced a new model of traffic on a uni-directional highway. In a recent manuscript [9] Greenberg studies an extension of this model, one which accounts for drivers attempting to travel at their maximum allowable speed. The author looks at a Lagrangian reformulation of this problem; a formulation that leads to an effective computational algorithm for solving the resulting system. He also investigates approximation scheme introduced by Dafermos and converges for scalar conservation laws and demonstrates that this Dafermos scheme works well on this 2×2 system.

Simulation of hysteresis and its analysis in magnetic and magnetoelastic systems

We study the simulation of the behavior of a magnetoelastic system under magnetic field loading. A detailed analysis of magnetic simulations is given in [10]. Our principle objective is to understand the magnetostrictive curve of Terfenol-D, $Tb_xDy_{1-x}Fe_2$, $x \approx 0.3$, from the viewpoint of micromagnetic theory. Simulations of magnetic, magnetostrictive, and pseudoelastic behavior exhibit hysteresis. These systems have a highly nonlinear character involving both short range anisotropy and elastic fields and dispersive demagnetization fields. The hysteretic character of a simple system that moves quasistatically is robust. The energy profile in terms of applied magnetic field, and in

particular, the width of the hysteresis loop, is invariant under mesh refinement. This is true even in the absence of an imposed dynamical mechanism, like the Landau-Lifschitz-Gilbert equation. This permits us, for example, to extract useful information by computing on fairly coarse grids. It is also very efficient. A typical simulation involves 600 to 800 field steps, each one of which represents a complete conjugate gradient iteration procedure.

An important feature of this type of simulation is that computed states are only metastable. Indeed, since the energy of configurations on loading and unloading are different for the same value of the imposed magnetic field, not both and usually neither can be minima. Little is known to guide us about metastability in this context. In addition, Terfenol displays a complicated lamellar microstructure whose role in the magnetostrictive process remains under investigation. Although confirming our ability to determine general features of the magnetization and magnetostriction, our results do not accurately describe the microstructure. So there is much room for improvement. However, we would like to point out that in our attempts to account for behavior of the growth twin midrib in our laminate, we witness a wave of magnetization reversal propagate across the domain. This is first evidence that we are able to achieve some progress here. Two sample figures are reproduced here.

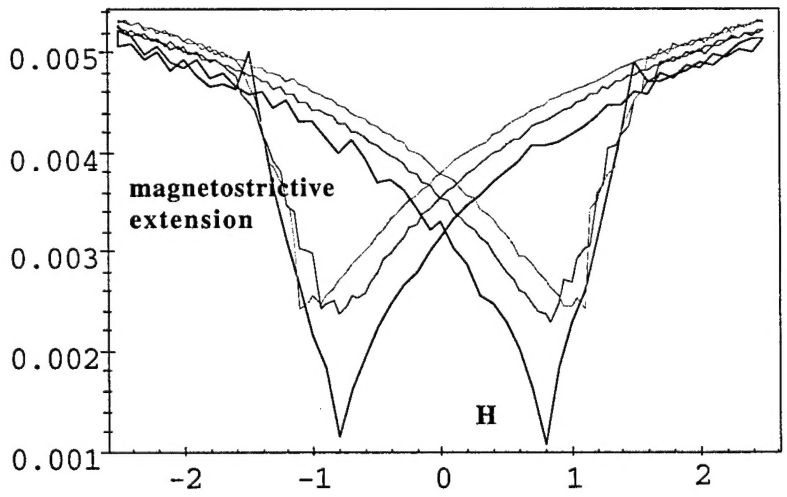


Figure 1. Magnetostriction curves: without demagnetization energy (lowest curve), single crystal with demagnetization energy (intermediate curve), and laminate with demagnetization energy (top curve).

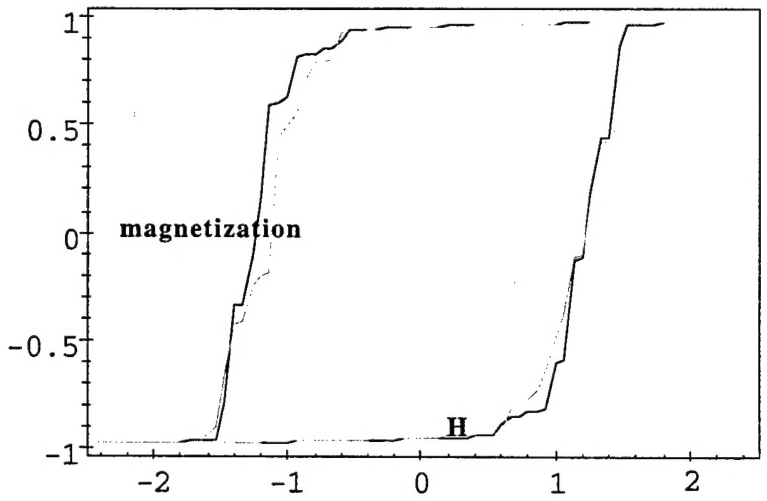


Figure 2. Magnetization curves for laminate (gray) and for laminate with constrained growth twin (black).

Mesoscale properties of polycrystalline materials with focus on the development of new techniques to resolve the grain boundary energy from experimental information.

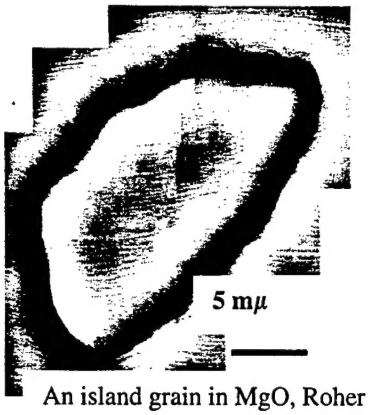
Almost all technologically useful materials are polycrystalline in nature, composed of a large number of grains of varying orientations separated by grain boundaries. Most failure mechanisms, like segregation, as well as many other properties are limited by the grain boundary properties. How can we describe this and do we have any hope of establishing predictive theoretical tools? What about the effects of dimensional reduction in thin films? The Mesoscale Interface Mapping Project is a joint project undertaken by Kinderlehrer and Ta'asan with colleagues in the Materials Science and Engineering Department led by Brent Adams. The main objectives of this project are to establish the grain boundary energy and mobility in several families of materials by use of orienting imaging microscopy.

Here we give a highlight of our results that illustrates how mesoscale methods can give rise to new information. An experimental technique using atomoc force microscopy and EBS (electron backscattered microscopy) has been developed to measure the surface energy anisotropy of crystalline solids. Observations are made at circumferential thermal grooves, the boundaries of island grains, where it is assumed that Herring's local equilibrium condition for a triple junction holds, giving rise to relations satisfied at points along circumference of the groove. Our objective is to reconstruct the surface energy from this information as an example of the statistical/multiscale method developed by Kinderlehrer, Mason, and their coworkers and described in a prior progess report.

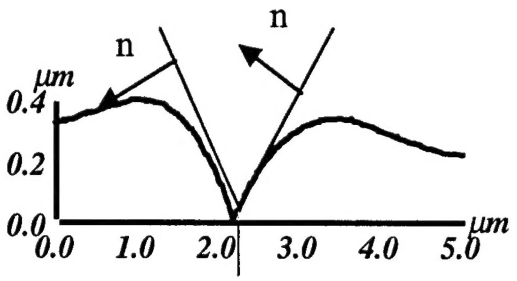
The equilibrium equations that hold along the groove, the Herring Relation or Young's Law, conform to the balance of forces between the surface energies of the island grain and the matrix and the grain boundary that separates the two. They have the form

$$\sum \left(\frac{\partial \sigma^{(i)}}{\partial \phi} n^{(i)} + \sigma^{(i)} t^{(i0)} \right) = - \sigma_{gb} e_3$$

where $\sigma^{(i)}$, i = a,b, is the surface energy evaluated on either side of the groove and σ_{gb} is the grain boundary energy. The $n^{(i)}$ and $t^{(i)}$ are assumed coplanar and ϕ is the angle in the common plane. The term $\partial\sigma^{(i)}/\partial\phi$ is referred to as a torque term. It has been an

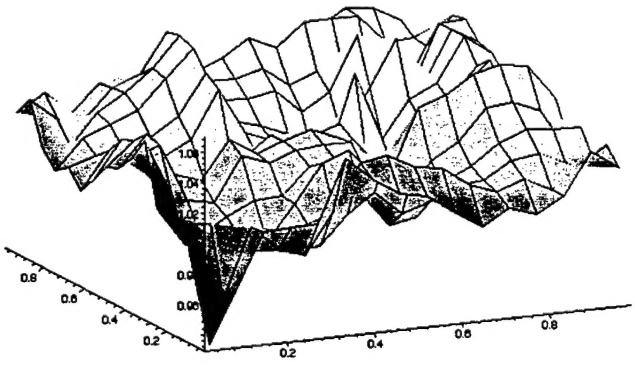


An island grain in MgO, Roher and Saylor

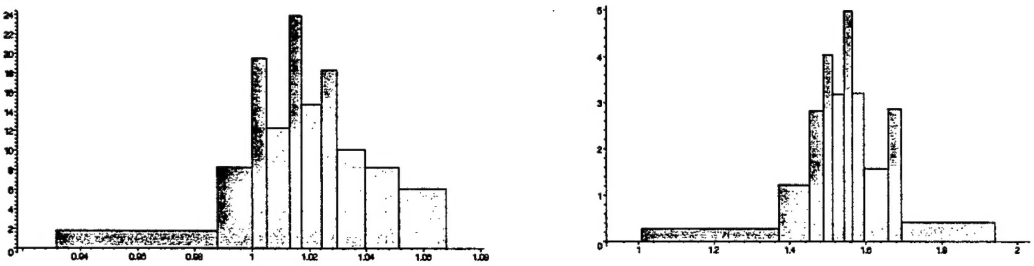


Groove geometry, Rohrer and Saylor

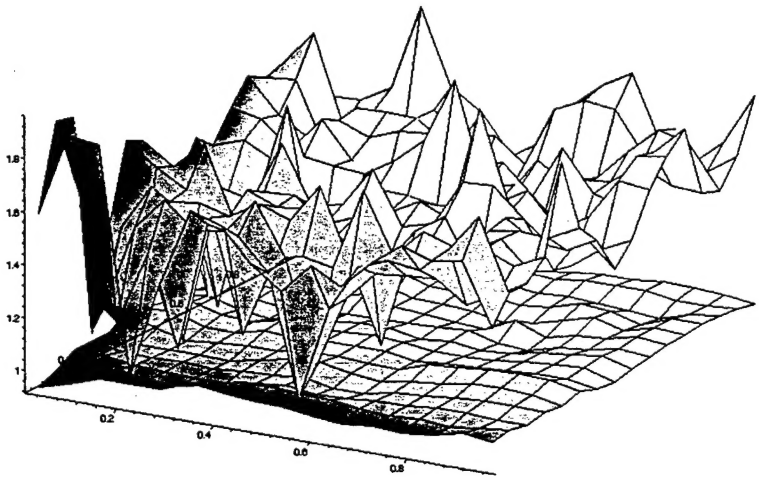
interesting open question to establish the significance of its role in the balance of forces. Do we see these torque terms or not in a this type of system? The traditional Wulff picture has only torque and no lattice mismatch, but it concerns crystal growth. The traditional Young's Law has only 'tension' . Here we are able to present first results that illustrate a dramatic role for the presence of torques. These are summarized in the pictures below.



Reconstruction of surface energy for MgO based on the Statistical/Multiscale technique (includes torque terms)
Depicted in crystallographic coordinates (hkl) with h = 1 and $0 \leq l,k \leq 1$



Histograms of energy values constructed with torque terms (left) and without torque terms (right). Note that the spread of values is much greater in the reconstruction without torque terms



Reconstructions of surface energy of magnesia employing torque terms in the Herring relation (below) and ignoring torque terms in the Herring relation (above). Note that ignoring torque terms leads to a reconstructed energy with much greater oscillation (greater anisotropy) and minima in unexpected places.

The first figure is a plot of the reconstruction of the energy function. The values show a range equal to about [1,1.1], with crystallographic direction (100) the minimum and (111) the maximum, approximately. These values conform to general expectations about MgO and provide, in addition, details of the energy that had not previously been available. We also performed a computation where the torque term is ignored. Here the range of values is about [1, 1.9], much greater. The two plots are shown together, which renders the energy with torques flat in comparison to the energy without torques. The histograms illustrate the dramatic difference in the spread of values. The standard deviations of the values are .02389265967 (with torque terms) and .1608315615 (without torque terms.)

The results suggest very strongly that the equilibrium of a thermal groove is substantially maintained by torques acting on the surface.

Mesoscale simulation of grain growth

Evolution of grain structure is the second focus of grain boundary processing. The theoretical and laboratory determination of parameters contributing to evolution is one of the challenges of our project. The evolution system for grain growth, here written for a columnar structure, has the form

$$v_n n = \mu \frac{d}{ds} T,\ T = \sigma'(\theta,\alpha)n + \sigma(\theta,\alpha)b,\ \text{on}\ \Gamma \qquad (1)$$

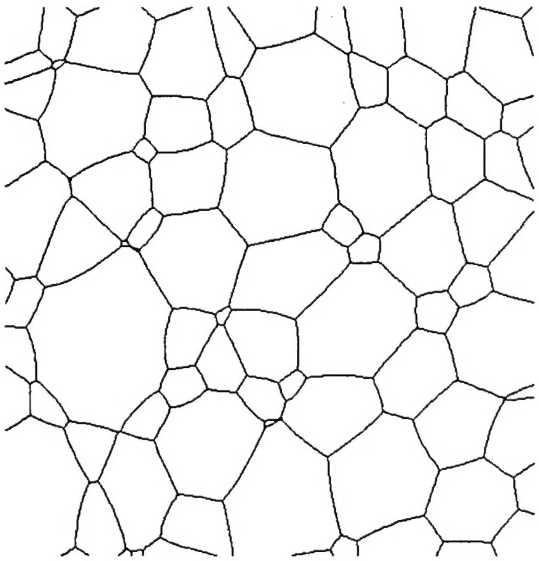
θ angle of normal vector n,	α lattice mismatch angle
b tangent vector	T stress vector of curve
v_n normal velocity of curve Γ	μ mobility (function of θ,α)

May we determine the parameters in the equation, especially the mobility μ? Whereas equilibrium demands a natural boundary condition at triple junctions, where the curves Γ meet, in evolution, a boundary condition must be assigned. We showed that the Herring Condition

$$\sum T^{(i)} = 0 \quad \text{at each triple junction}$$

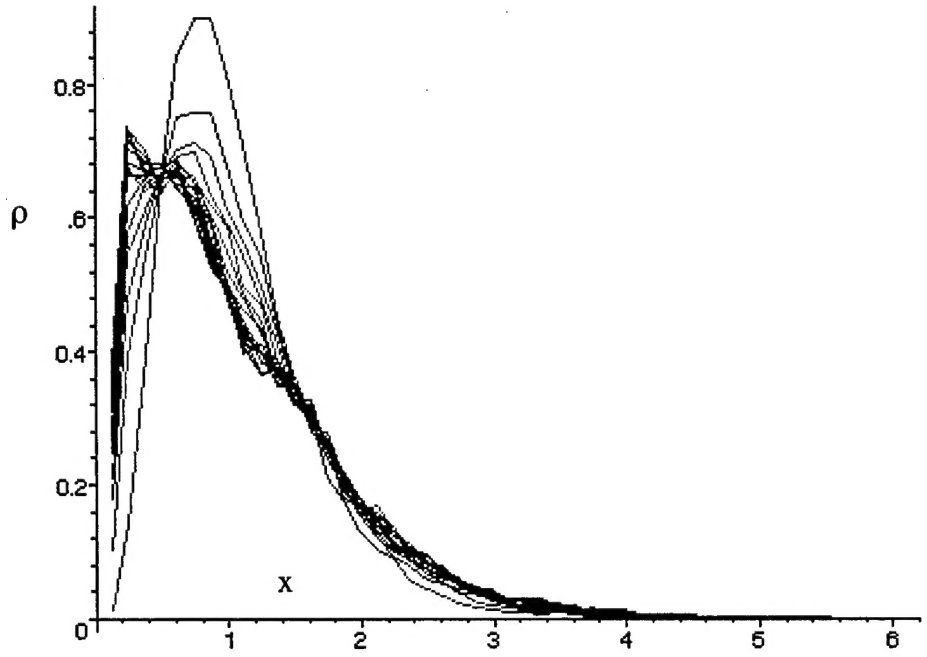
the natural boundary condition for equilibrium ensures that the dynamical system is dissipative. Initial configurations close to equilibrium configurations evolve to an equilibrium configuration, although not necessarily the one they started close to.

There are fundamental issues of information associated to the simulation of a large metastable system comprising many independent and only weakly communicating elements. The simplest of these is what such a simulation predicts. Unlike the calculation of an airflow where velocities and pressures are direct results of the calculation, the properties of an initial configuration that gives rise to the properties of the final configuration concerning distribution of grain sizes, orientations, amounts of grain boundary, etc. are necessarily statistical in nature. We do not have methods available for the resolution of this issue. We are currently working with Anthony Kearsely, Anthony Rollett, and Shlomo Ta'asan on the development methods to address this issue.



An intermendiate stage in the evolution

We have begun simulation of curvature driven growth to explore these fundamental issues. Here we address the mesoscale simulation of large systems of grain boundaries subject to the Mullins equation of curvature driven growth with the Herring force balance equation imposed at triple junctions, as described above. There are several novel features of our apporach which we anticipate will render it a flexible, scalable, and robust tool to aid in microstructural prediction. At present the results are for two dimensional configurations. In this type of simulation, from our viewpoint the problem becomes one of solving a large system of evolution equations subject to complementing boundary conditions, metastable but always dissipative. In our technique we are able to track large numbers of grains (e.g., up to 25,000) by simulating the evolution of the network of curves constituting grain boundaries, a data structure of dimensionality one less than that of the grains themselves. A number of algorithmic innovations enhance both accuracy and speed. Two basic types of critical events can occur. When a grain side is collapsed, a four-junction temporarily forms and must be split into two triple junctions in a stable way. When a grain becomes too small, it must be absorbed into one of its neighbors. Rules for these events are part of the simulation. We computed the relative histograms $\rho(x,t)$, x = area/<area> at time t. The plots below indicate that these densities exhibit a surprising self-similarity



Relative histograms over at time steps 1 –16x1000 from a 25,000 grain simulation. Other simulations showed nearly identical histograms

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Mason

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